Diisopropyl fluorophosphate

55-91-4 | DTXSID1040667

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 195 °C

Global applicability domain: Inside

Local applicability domain index: 6.16e-01

Confidence level: 6.91e-01

Nearest Neighbors from the Training Set

Image not found
Diisopropyl fluorophosphate
Measured: 183
Predicted: 195

Image not found
Triethyl phosphate
Measured: 216
Predicted: 211

Image not found
Cyclosarin
Measured: 239
Predicted: 216

Image not found
Diethyl ethylphosphonate
Measured: 198
Predicted: 196

Image not found
Pinacolyl
methylphosphonofluoridate
Measured: 198
Predicted: 201